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Is there relevance of chaos in numerical solutions of quantum billiards?

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Abstract. In numerically solving the Helmholtz equation inside a connected plane domain with Dirichlet boundary conditions (the problem of the quantum billiard) one surprisingly faces enormous difficulties if the domain has a problematic geometry such as various nonconvex shapes. We have tested several general numerical methods in solving the quantum billiards. Following our previous paper (Li and Robnik 1995) where we analyzed the Boundary Integral Method (BIM), in the present paper we investigate systematically the so-called Plane Wave Decomposition Method (PWDM) introduced and advocated by Heller (1984, 1991). In contradistinction to BIM we find that in PWDM the classical chaos is definitely relevant for the numerical accuracy at fixed density of discretization on the boundary b (b = number of numerical nodes on the boundary within one de Broglie wavelength). This can be understood qualitatively and is illustrated for three one-parameter families of billiards, namely Robnik billiard, Bunimovich stadium and Sinai billiard. We present evidence that it is not only the ergodicity which matters, but also the Lyapunov exponents and Kolmogorov entropy. Although we have no quantitative theory we believe that this phenomenon is one manifestation of quantum chaos.

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1 Introduction

It is quite embarrassing to realize that in an attempt to numerically solve the Helmholtz equation

$$\nabla^2_{\mathbf{r}}\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = 0, \tag{1}$$

satisfied by the scalar solution $\psi(\mathbf{r})$ with eigenenergy $E = k^2$ inside a connected plane domain $\mathcal{B}$ with the Dirichlet boundary condition $\psi(\mathbf{r}) = 0$ on the boundary $\partial\mathcal{B}$, one can face enormous difficulties in cases of "problematic" geometries such as e.g. various nonconvex shapes. This is precisely the problem of solving and describing the quantum billiard $\mathcal{B}$ as a Hamiltonian dynamical system, which is thus just the 2-dim Schrödinger problem for a free point particle moving inside the enclosure $\partial\mathcal{B}$, described by the wavefunction $\psi(\mathbf{r})$ with the eigenenergy $E = k^2$. The corresponding classical problem is the classical dynamics of a freely moving point particle obeying the law of specular reflection upon hitting the boundary $\partial\mathcal{B}$. Quantum billiards and their correspondence to their classical counterparts, especially in the semiclassical level, are important model systems in studies of quantum chaos (Gutzwiller 1990, Giannoni *et al* 1991). There are several *general* methods for a numerical solution of equation (1) such as the Boundary Integral Method (BIM), recently carefully and extensively studied by Li and Robnik (1995a), following the important paper by Berry and Wilkinson (1984) (see also Boasman 1994), and the Plane Wave Decomposition Method (PWDM), introduced and advocated by Heller (1984,1991), whose analysis — especially in the light of the relevance of classical chaos — is the subject of our present paper. Another quite general method is the conformal mapping diagonalization technique introduced by Robnik (1984) and further developed by Berry and Robnik (1986) and recently by Prosen and Robnik (1993,1994), which in principle works for any shape whereas in practice it is used for shapes for which the conformal mapping onto the unit disk[3] is sufficiently simple (possiblly also analytic). These methods can face quite similar problems in cases of almost intractable geometries, but they are to some extent complementary. For example, the conformal mapping diagonalization technique can provide a complete set of all eigenenergies up to some maximal value beyond which the calculations cannot be performed due to the lack of computer storage (RAM), which means that we cannot reach very high-lying eigenstates.

[3]or some other integrable geometries admitting a simple basis for the representation

(Our present record (Prosen and Robnik 1994) is about 35,000 for the size of the banded matrix that we diagonalize in double precision, yielding at least 12,000 good levels with accuracy of at least one percent of the mean level spacing.)

However, using PWDM it is possible to go higher in energy by orders of magnitude but then only a few selected states can be calculated with many intermediate states in the spectral stretch missing. Therefore the geometry of some interesting and representative high-lying states can be analyzed, but the sample is typically not sufficiently complete (many missing states) to perform statistical analysis. See e.g. our recent papers on this topics (Li and Robnik 1994a, 1995b, 1995c, 1995d). The reasons for a failure of one of these methods can be quite different. For example, in BIM the main difficulty stems from the existence of "exterior chords" in nonconvex geometries in its standard formulation, but the trouble might be overcome by an appropriate reformulation of the method adapted to the correct semiclassical behaviour. This is discussed in (Li and Robnik 1995a) where we also show that classical chaos is completely irrelevant for BIM. On the contrary, in PWDM we find that the classical chaos is relevant for numerical accuracy especially in the semiclassical limit of sufficiently small effective Planck constant $\hbar_{eff}$ reached at sufficiently high eigenenergies. This demonstration and its qualitative explanation is the main subject of our present paper. To give a specific example we should mention isospectral billiards discovered and proved by Gordon *et al* (1992) which have been investigated experimentally (Sridhar and Kudrolli 1994) and it is also our experience (Li and Robnik 1994b) that BIM fails completely in this case (namely, due to strong nonconvexities) whereas PWDM at $b = 12$ yields the accuracy of eigenenergies of about within a few percent of the mean level spacing, except for some very special eigenmodes for which surprisingly we find agreement within double precision (16 digits) and which are characterized by the fact that these eigenvalues agree with the analytic solutions for the triangles within single precision (8 digits). So the fact that in this and similar cases the experimental precision (for some levels) exceeds the best possible numerical precision even when using the best available methods is embarrassing for a theoretician but also motivation for further work.

2 The plane wave decomposition method of Heller

In this section we present our general exposition of PWDM following Li and Robnik (1994a). To solve the Schrödinger equation (1) for $\psi(\mathbf{r})$ with Dirichlet boundary condition $\psi(\mathbf{r}) = 0$ on $\partial\mathcal{B}$ we use the *Ansatz* of the following superposition of plane waves (originally due to Heller (1984))

$$\psi(\mathbf{r}) = \sum_{j=1}^{N} a_j \cos(k_{xj}x + k_{yj}y + \phi_j), \tag{2}$$

where $k_{xj} = k\cos\theta_j$, $k_{yj} = k\sin\theta_j$, $k^2 = E$, and we use the notation $\mathbf{r} = (x, y)$. N is the number of plane waves and ϕ_j are *random phases*, drawn from the interval $[0, 2\pi)$, assuming uniform distribution, and $\theta_j = 2j\pi/N$ determining the direction angles of the wavevectors chosen equidistantly. The *Ansatz* (2) solves the Schrödinger equation (1) in the interior of the billiard region $\mathcal{B}$, so that we have only to satisfy the Dirichlet boundary condition. Taking the random phases, as we discovered, is equivalent to spreading the origins of plane waves all over the billiard region, and at the same time this results in reducing the CPU-time by almost a factor of ten. For a given k we put the wavefunction equal to zero at a finite number M of boundary points (primary nodes) and equal to 1 at an arbitrarily chosen interior point. Of course, $M \geq N$. This gives an inhomogeneous set of equations which can be solved by matrix inversion. Usually the matrix is very singular, thus the *Singular Value Decomposition* (SVD) method has been invoked (Heller 1984, Press *et al* 1986). After obtaining the coefficients a_j we calculate the wavefunctions at other boundary points (secondary nodes). We always have 3 secondary nodes between a pair of primary nodes. The experience shows that further increase of the number of secondary nodes does not enhance the accuracy. The sum of the squares of the wavefunction at all the secondary nodes (Heller called this sum "tension") would be ideally zero if k^2 is an eigenvalue and if (2) is the corresponding exact solution of (1). In practice it is a positive number. Therefore the eigenvalue problem now is to find the minimum of the "tension". In our numerical procedure we have looked for the zeros of the first derivative of the tension; namely the derivative is available analytically/explicitly from (2) once the amplitudes a_j have been found. In this paper we make the choice $M = N$, since it proved to be sufficient for

calculating the lowest 100 states whose accuracy we analyze. (For high-lying states studied in (Li and Robnik 1994a) we have used $M = 5N/3$.) It must be pointed out that the wavefunctions obtained in this way are not (yet) normalized, due to the arbitrary choice of the interior point where the value of the wavefunction has been arbitrarily set equal to unity. We therefore explicitly normalize these wave functions before embarking to the analysis of their properties.

The accuracy of this method of course depends on the number of plane waves (N) and on the number of the primary nodes (M), and we have a considerable freedom in choosing N and $M \geq N$. In order to reach a sufficient accuracy the experience shows that we should take at least $N = 3\mathcal{L}/\lambda_{deBroglie}$, and $M = N$, where $\mathcal{L}$ is the perimeter of the billiard and $\lambda_{deBroglie}$ is the de Broglie wavelength $= 2\pi/k$. With this choice in the present context and for the lowest 100 states we reach the double precision accuracy (sixteen digits) for all levels of integrable systems like rectangular billiard (where the eigenenergies can be given trivially analytically) and the circular billiard, but also for Robnik billiard $\mathcal{B}_\lambda$ for small $\lambda \leq 0.1$. Introducing the density of discretization b defined as the number of numerical nodes per one de Broglie wavelength on the boundary we thus write the number of plane waves $N = b\mathcal{L}/\lambda_{deBroglie} = b2\pi\mathcal{L}/k$.

The main problem of investigation in this paper is to study the dependence of the systematical numerical error ΔE (i.e. the error due to the finite discretization) on the density of discretization b, and the dependence of ΔE on the geometry (billiard shape parameter) at fixed b. In order to perform a systematic analysis the errors should be measured in some natural units and in our case this is of course just the mean level spacing which according to the leading term of Weyl formula is equal to $4\pi/\mathcal{A}$ where $\mathcal{A}$ is the area of the billiard $\mathcal{B}$. From now on we shall always assume that ΔE of a particular energy level is in fact measured in such natural units. Of course one immediately realizes that the error ΔE fluctuates wildly from state to state (see figure 5) so that generally nothing can be predicted about it individually. Therefore the approach must be a statistical one and so we typically take an average of the errors ΔE over a suitable ensemble of states. Specifically, in all cases of this paper we have taken the average of the absolute values of ΔE over the lowest 100 states (of a given symmetry class) and denote

it by $< |\Delta E| >$. It is important and should be mentioned that we have also checked the stationarity of such average value over consecutive spectral stretches of 100 states each, so that our procedure does make sense. See a discussion at the end of section 3.

It turns out that the accuracy of energy levels depends nontrivially on b, unlike in BIM (where we find always a power law (Li and Robnik 1995a)), namely it typically shows broken power law. By this we mean that $< |\Delta E| >$obeys a power law $< |\Delta E| >= Ab^{-\alpha}$ with very large α for sufficiently small b, $b \leq b_c$, whereas for larger $b \geq b_c$ it obeys a rather flat power law with very small positive α (close to zero). Therefore in contradistinction to BIM it is difficult to explore the general dependence of $< |\Delta E| >$on b, if there is any such universality at all. However, in order to investigate the dependence of the accuracy on geometry and the implied dynamical properties of billiards, we have decided to fix the value of b and have chosen $b = 12$, and then we look at the dependence of $< |\Delta E| >$on the shape parameters of three one-parameter billiards, namely Robnik billiard, Bunimovich stadium and Sinai billiard.

3 Numerical results

As is well known in classically integrable quantum Hamiltonian systems in the semiclassical limit (of sufficiently small $\hbar$) the eigenfunction can locally be described by a *finite* superposition of plane waves with the same wavenumber, in case of plane billiards it is $k = \sqrt{E}$. If the quantum system has ergodic classical dynamics then in the semiclassical limit locally the wavefunction can be represented as a superposition of *infinitely* many plane waves with the same k and with the wavevectors being isotropically distributed on the circle of radius k. Moreover, the ergodicity suggests to assume random phases for the ensemble of plane waves which implies that to the lowest approximation the wavefunction is a Gaussian random function. While this is a good starting approximation, originally due to Berry (1977) and recently verified by Aurich and Steiner (1993) and also by Li and Robnik (1994a), the phases are actually not random but correlated in a subtle way dictated by the classical dynamics especially along the short and the least unstable periodic orbits, which is the origin of the scar phenomenon (Heller 1984,

1991, Bogomolny 1988, Berry 1989, Robnik 1989, Li and Robnik 1995d). (For a discussion see (Robnik 1988, 1995).) Thus we can qualitatively very well understand that PWDM should work well or even brilliantly in cases of classically integrable billiards whereas in the ergodic systems we expect a severe degradation of the accuracy (at fixed b) simply because the finite number of plane waves cannot capture the correct (infinite) superposition of plane waves everywhere in the interior of the billiard. If the system is a generic system of a mixed type with regular and irregular regions coexisting in the classical phase space, a scenario described by the KAM theory, then the degradation of accuracy (at fixed b) with increasing fractional measure of the chaotic component (denoted by ρ_2) is certainly expected. However, ρ_2 is not the only parameter which controls the accuracy (at fixed b), since, as we shall see, the dynamical properties like diffusion time, Lyapunov exponent and the Kolmogorov entropy play a role. It is the aim of the present paper to numerically explore this type of behaviour in three different billiard systems.

The first billiard system is defined as the quadratic (complex) conformal map $w = z + \lambda z^2$ from the unit disk $|z| \leq 1$ from the z plane onto the $w = (x, y)$ complex plane. The system has been introduced by Robnik (1983) and further studied by Hayli *et al* (1987), Frisk (1990), Bruus and Stone (1994) and Stone and Bruus (1993a,b) for various parameter values λ. Since the billiard (usually called Robnik billiard) has analytic boundary it goes continuously from integrable case (circle, $\lambda = 0$) through a KAM-like regime of small $\lambda \leq 1/4$ with mixed classical dynamics, becomes nonconvex at $\lambda = 1/4$ (the bounce map becomes discontinuous), where the Lazutkin caustics (invariant tori) are destroyed giving way to ergodicity. As shown by Robnik (1983) the classical dynamics at these values of λ is predominantly chaotic (almost ergodic), although Hayli *et al* (1987) have shown that there are still some stable periodic orbits surrounded by very tiny stability islands up to $\lambda = 0.2791$. At larger λ we have reason and numerical evidence (Li and Robnik 1994c) to expect that the dynamics can be ergodic. It has been recently rigorously proven by Markarian (1993) that for $\lambda = 1/2$ (cardioid billiard) the system is indeed ergodic, mixing and K. This was a further motivation to study the cardioid billiard classically, semiclassically and quantanlly by several groups e.g. by Bäcker *et al* (1994) and Bäcker (1995), Bruus and Whelan (1995). The billiard shape for $\lambda = 0.4$ is shown (the upper half) in figure 1a. Since all states are either even or odd we can take into account these symmetry

properties explicitly. In fact we want to specialize to the odd eigenstates only. Therefore in order to a priori satisfy the Dirichlet boundary condition on the abscissa of figure 1a we specialize the general *Ansatz* (2) to the following form

$$\psi(\mathbf{r}) = \sum_{j=1}^{N} a_j \cos(k_{xj}x + \phi_j) \sin(k_{yj}y), \tag{3}$$

where all the quantities are precisely as in (2) except that the N discretization (primary) nodes are equidistantly located only along the half of the full billiard boundary, so that b is exactly the same as in using the *Ansatz* (2) for the full billiard.

In figure 2 we show the results for this billiard, namely we plot $< |\Delta E| >$versus λ at fixed $b = 12$. Close to integrability ($\lambda \leq 0.1$) we reach the accuracy within 14 to 15 digits which is almost the double precision on our machine (16 digits), in which all our calculations have been performed. As the value of λ increases we observe a dramatic deterioration of the accuracy where $< |\Delta E| >$increases by many orders of magnitude, namely almost by 13 decades, leveling off at $< |\Delta E| >$approximately equal to 10^{-2}, which means that we have now the accuracy of only a few percent of the mean level spacing. This dramatic but quite smooth increase of $< |\Delta E| >$is certainly related to the emergence of classical chaos with increasing λ, but definitely is *not* controlled merely by ρ_2, because ρ_2 reaches the value of 1 (almost ergodicity) already at $\lambda = 1/4$ (Robnik 1983, Prosen and Robnik 1993), whereas $< |\Delta E| >$still varies considerably in the region $\lambda \geq 1/4$. Thus it is obvious that in the semiclassical picture also other classical dynamical properties (measures of the "hardness" of chaos) play an important role. Although we do not have a quantitative theory yet one should observe that according to (Robnik 1983) the Lyapunov exponent and Kolmogorov entropy (h) vary also quite smoothly with λ, suggesting a speculation that there might be a relation between $< |\Delta E| >$and h.

Another demonstration of the effectivity of PWDM and its accuracy is displayed in table 1 where we show the numerical value of the scalar product of two consecutive normalized eigenstates, namely the ground state and the first excited state, denoted by O_{12}, which ideally should be zero. As we see here too the accuracy decreases (by orders of magnitude) sharply but smoothly

with increasing shape parameter λ.

It is then interesting to similarly analyze an ergodic system such as stadium of Bunimovich shown in figure 1b, where the shape parameter is a/R and we have looked at the results for $0 \leq a/R \leq 10$. In fact for our purposes we have chosen and fixed $R = 1$ in all cases. Since this billiard is known to be rigorously ergodic (and mixing and K) for any $a > 0$ in this case ρ_2 is exactly 1 and constant. We have calculated the lowest 100 energy levels of the odd-odd symmetry class. Therefore in this case the general *Ansatz* (2) can be specialized as follows

$$\psi(\mathbf{r}) = \sum_{j=1}^{N} a_j \sin(k_{xj}x) \sin(k_{yj}y). \tag{4}$$

Here again the discretization (primary) nodes are only on the outer boundary of the stadium with discretization density $b = 12$. From our plot in figure 2 we see that in the integrable case of the circle ($a = 0$) we again reach the accuracy within at least 14 digits, but this brilliant accuracy at fixed $b = 12$ deteriorates almost discontinuously upon increasing a and then $< |\Delta E| >$still increases by about two orders of magnitude when a goes from 0.1 to 10. It appears to us that classical chaos is definitely relevant for the accuracy of the method which might and should be explained by an appropriate theory in the semiclassical level. As an observation we should mention that the Kolmogorov entropy increases sharply with a/R when a/R goes from 0 to about 1, where it reaches the maximum, and then decreases slowly (Benettin and Strelcyn 1978), whereas our $< |\Delta E| >$increases monotonically. Thus if there is a relationship between $< |\Delta E| >$and Kolmogorov entropy it certainly is not a simple one.

We have tested also another system with hard chaos, namely the Sinai billiard sketched in figure 1c (desymmetrized). The system is known to be ergodic, mixing and K. In calculating the 100 lowest energy levels of the desymmetrized Sinai billiard we used the same specialized *Ansatz* as in eq. (3), thereby taking into account explicitly the Dirichlet boundary condition on the abscissa $y = 0$. In this case b is the density of discretization of the equidistant nodes along the rest of the perimeter. Similarly as in case of stadium we easily reach the double precision of 16 digits in the limiting integrable case of zero radius $R = 0$, but this accuracy is almost instantly lost

by increasing R as seen in figure 3. The value of $< |\Delta E| >$levels off at about 10^{-3} to 10^{-2} for all R between 0.025 and 0.45.

As a final technical point we comment on the stationarity of $< |\Delta E| >$as a function of energy, which has been confirmed for the Robnik billiard at $\lambda = 0.27$ where the average value over consecutive spectral stretches over 100 states has been found to be quite stable. Specifically, to illustrate this finding we plot in figure 5 the absolute values of the lowest 400 consecutive eigenstates where one can see that the average value over 100 consecutive states is quite stable indeed. This is shown in table 2 for four intevals of 100 states each.

4 Discussion and conclusions

We believe that our present paper presents quite firm numerical (phenomenological) evidence for the relevance of classical chaos for the effectiveness of PWDM as a quantal numerical method to solve a quantum billiard, which is manifested especially in the semiclassical limit and might and should be explained in terms of an appropriate semiclassical theory. Qualitatively the reasons for this phenomenon are explained in the first paragraph of section 3. The parameter ρ_2 (the fractional volume of the chaotic component(s)) definitely plays an important role but is not the only aspect of classical chaos controlling the behavior of the error $< |\Delta E| >$at fixed discretization density b. Namely even in rigorously ergodic systems where ρ_2 is 1 the error $< |\Delta E| >$might be controlled by the slow diffusion in the classical phase space (diffusive ergodic regime, soft chaos). If the classical diffusion time is much longer than the break time t_{break} ($t_{break} = \hbar/D$, D = mean energy level spacing) then the quantal states will be strongly localized in spite of the formal ergodicity (for a demonstration see (Li and Robnik 1995b)), and therefore they mimic certain amount of regularity enabling a better accuracy of PWDM, i.e. $< |\Delta E| >$is smaller than for completely extended chaotic high-lying eigenstates where according to our experience somehow $< |\Delta E| >$typically saturates at about a few percent of the mean level spacing, even if we brutally increase b beyond any reasonable limits. Indeed, as can be seen by comparison of figures 2, 3 and 4, in case of the stadium this saturation value of $< |\Delta E| >$is about 10^{-4}, which is almost two orders of

magnitude smaller than in the Sinai billiard (figure 4) and cardioid billiard (figure 2). We think that this is due to the strong localization of eigenstates in the stadium, which is very well known to display an unusual abundance of scars (Heller 1984, Li and Robnik 1995d).

Thus our present work is a motivation for a semiclassical theory to explain this aspect of quantum chaos which exhibits some algorithmical properties of PWDM in applying it to quantum billiards with variety of classical dynamics.

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Tables

Table 1. The test of the orthogonality of the eigenstates. The scalar product of two consecutive normalized wavefunctions O_{12}, namely the ground state and the first excited state, for Robnik billiard at different shape parameters.

λ	O_{12}
0	2.0E−16
0.1	-5.0E−15
0.2	7.8E−10
0.3	4.8E−6
0.4	5.5E−4
0.5	1.5E−3

Table 2. The stationarity test of $< |\Delta E| >$for Robnik billiard at $\lambda = 0.27$ for the lowest 400 odd eigenstates.

average stretch	$< \|\Delta E\| >$
1-100	1.54E−7
101-200	2.21E−7
201-300	2.77E−7
301-400	2.03E−7
1-400	2.13E−7

Figure captions

Figure 1 (a-c): The geometry of the boundary of the three desymmetrized billiards, the Robnik billiard (a), the Bunimovich stadium (b) and the Sinai billiard (c).

Figure 2: The ensemble averaged (over 100 lowest odd eigenstates) absolute error (measured in units of mean level spacing) versus the billiard shape parameter λ for Robnik billiard with fixed density of boundary discretization $b = 12$. The numerical points are denoted by the diamonds, which are joined by straight lines just to guide the eye.

Figure 3: The ensemble averaged (over 100 lowest odd-odd eigenstates) absolute error (measured in units of mean level spacing) versus the billiard shape parameter a/R for Bunimovich stadium with fixed density of boundary discretization $b = 12$. The numerical points are denoted by the diamonds, which are joined by straight lines just to guide the eye.

Figure 4: The ensemble averaged (over 100 lowest eigenstates) absolute error (measured in units of mean level spacing) versus the billiard parameter R (the radius of inner circle) for the desymmetrized Sinai billiard with fixed density of boundary discretization $b = 12$. The numerical points are denoted by the diamonds, which are joined by straight lines just to guide the eye.

Figure 5: The absolute error of eigenstates versus eigenenergy for the lowest 400 odd eigenstates of Robnik billiard at $\lambda = 0.27$. The averages over consecutive stretches (of 100 states each) are given in table 2, demonstrating that $< |\Delta E| >$is quite stationary.

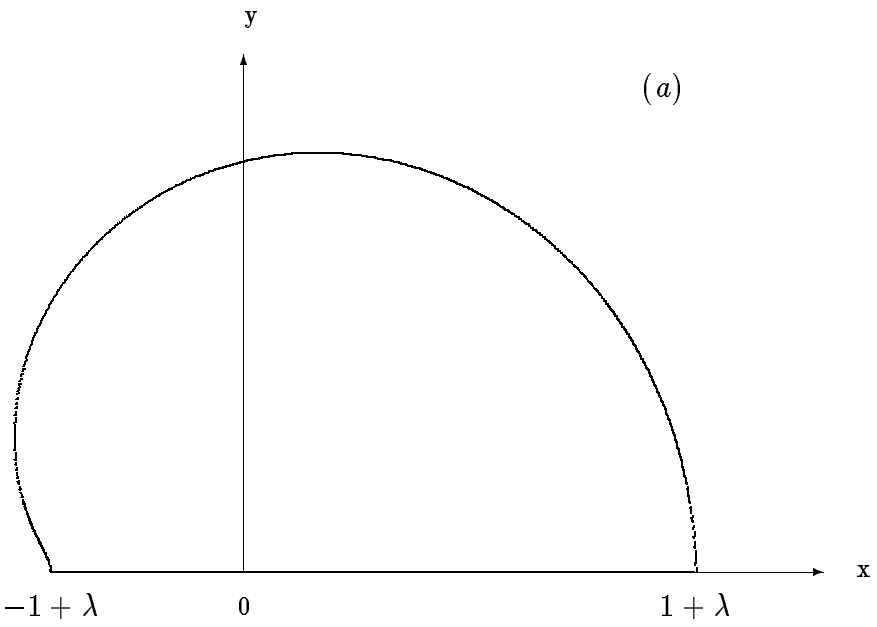


Figure 1

Figure 1

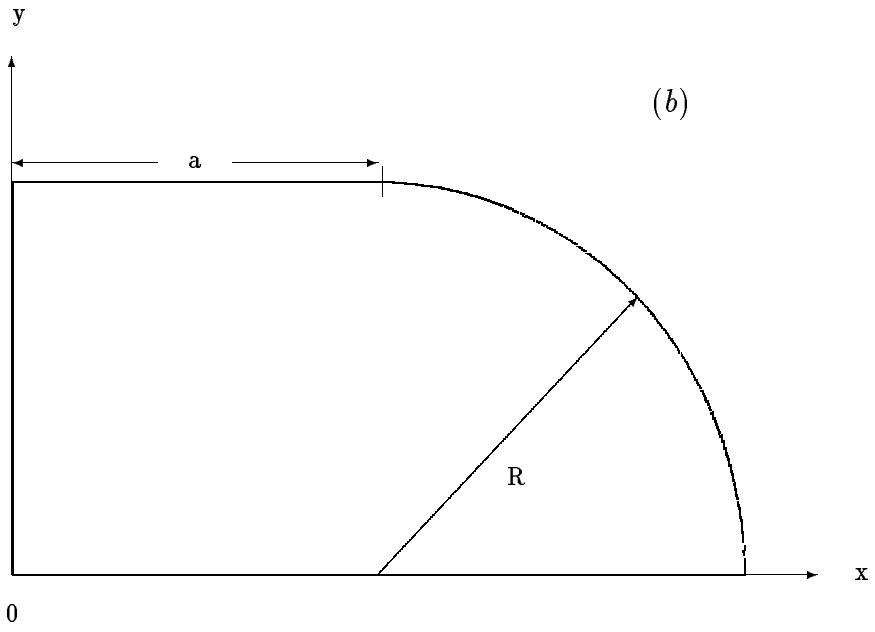


Figure 1

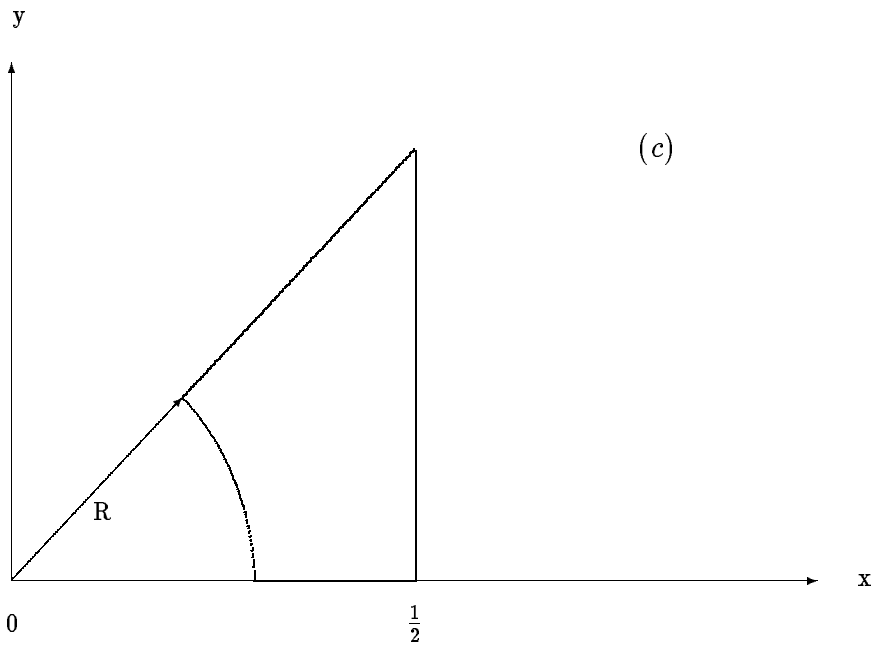


Figure 2

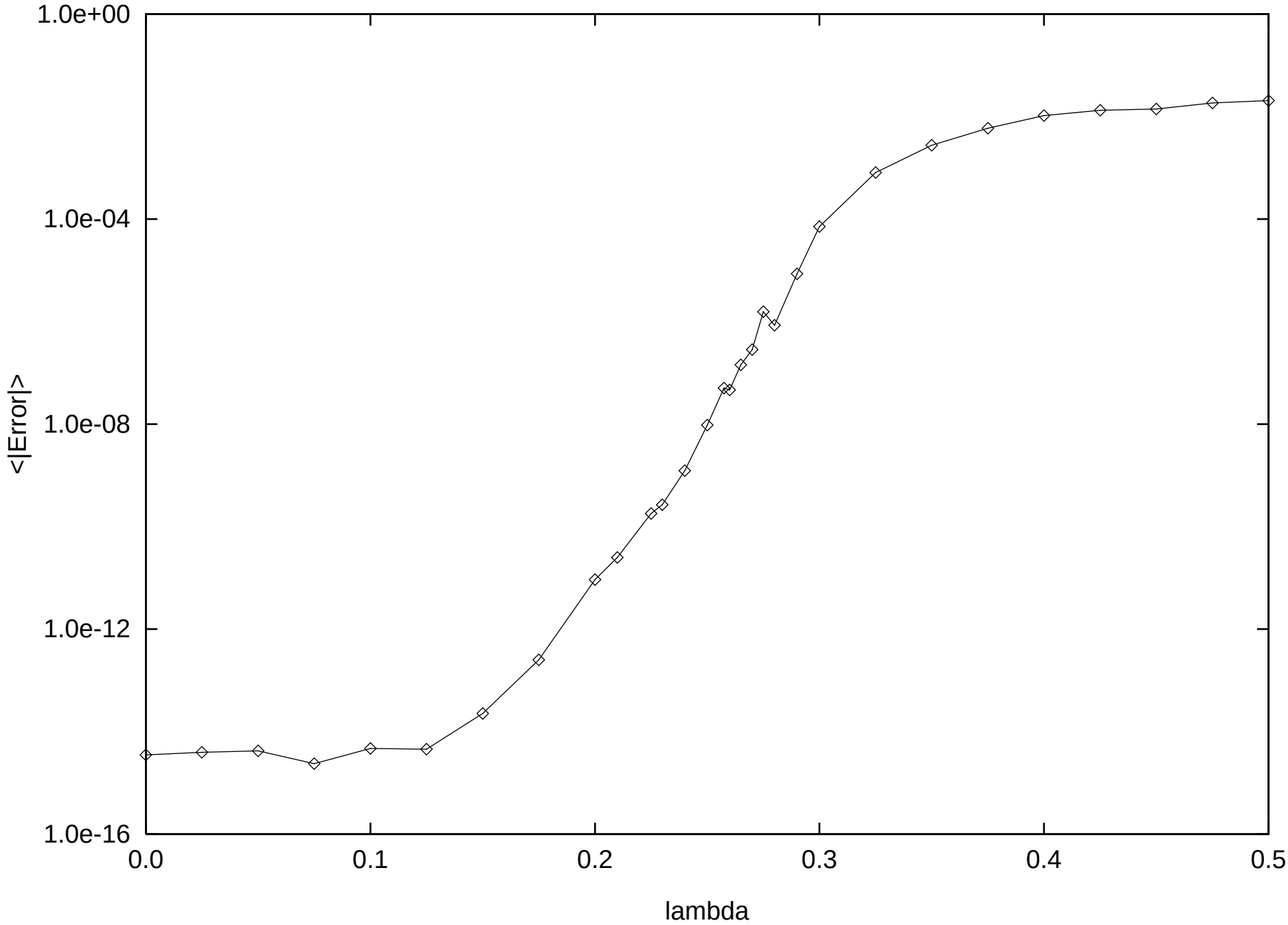
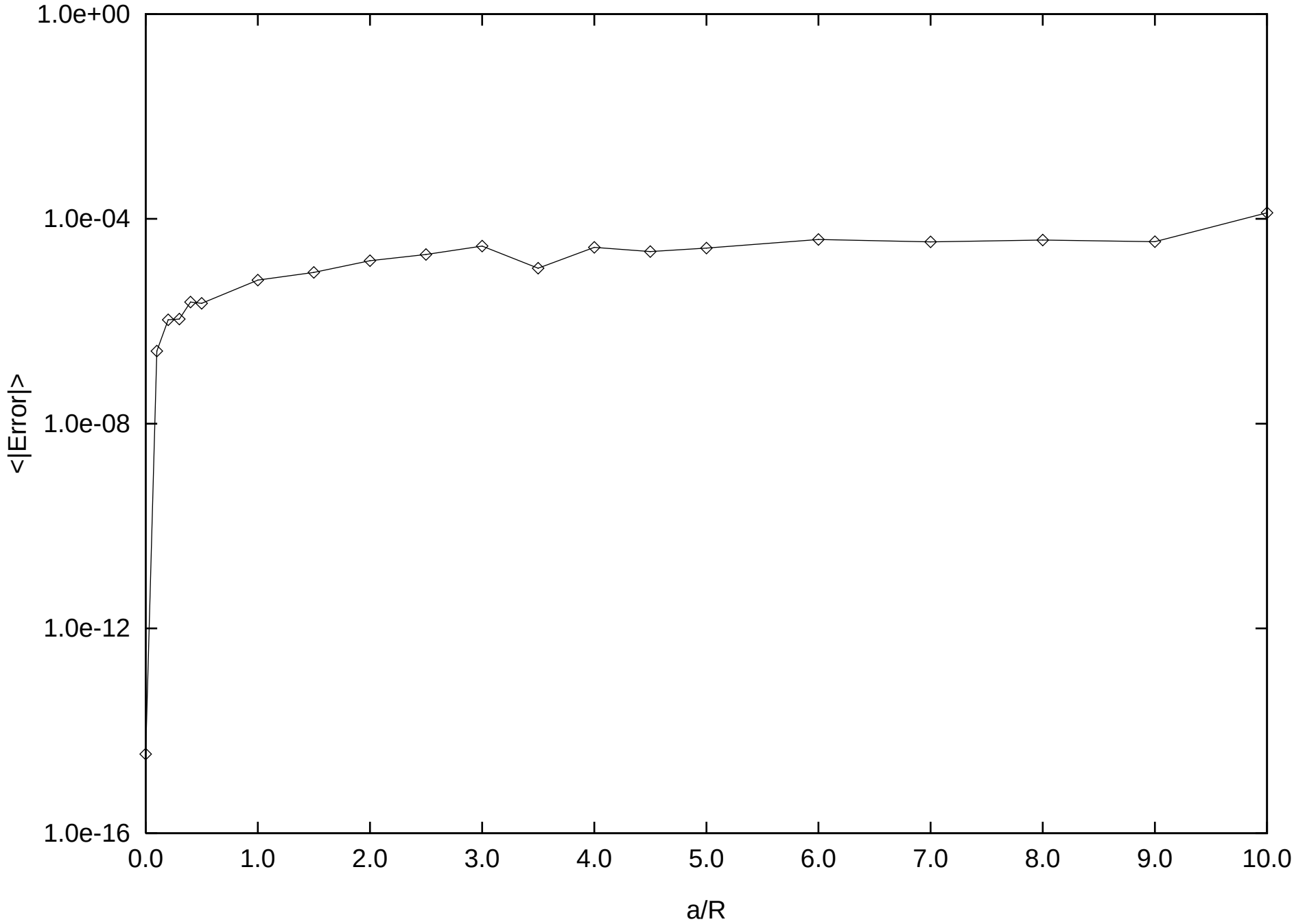


Figure 3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a/R

Figure 4

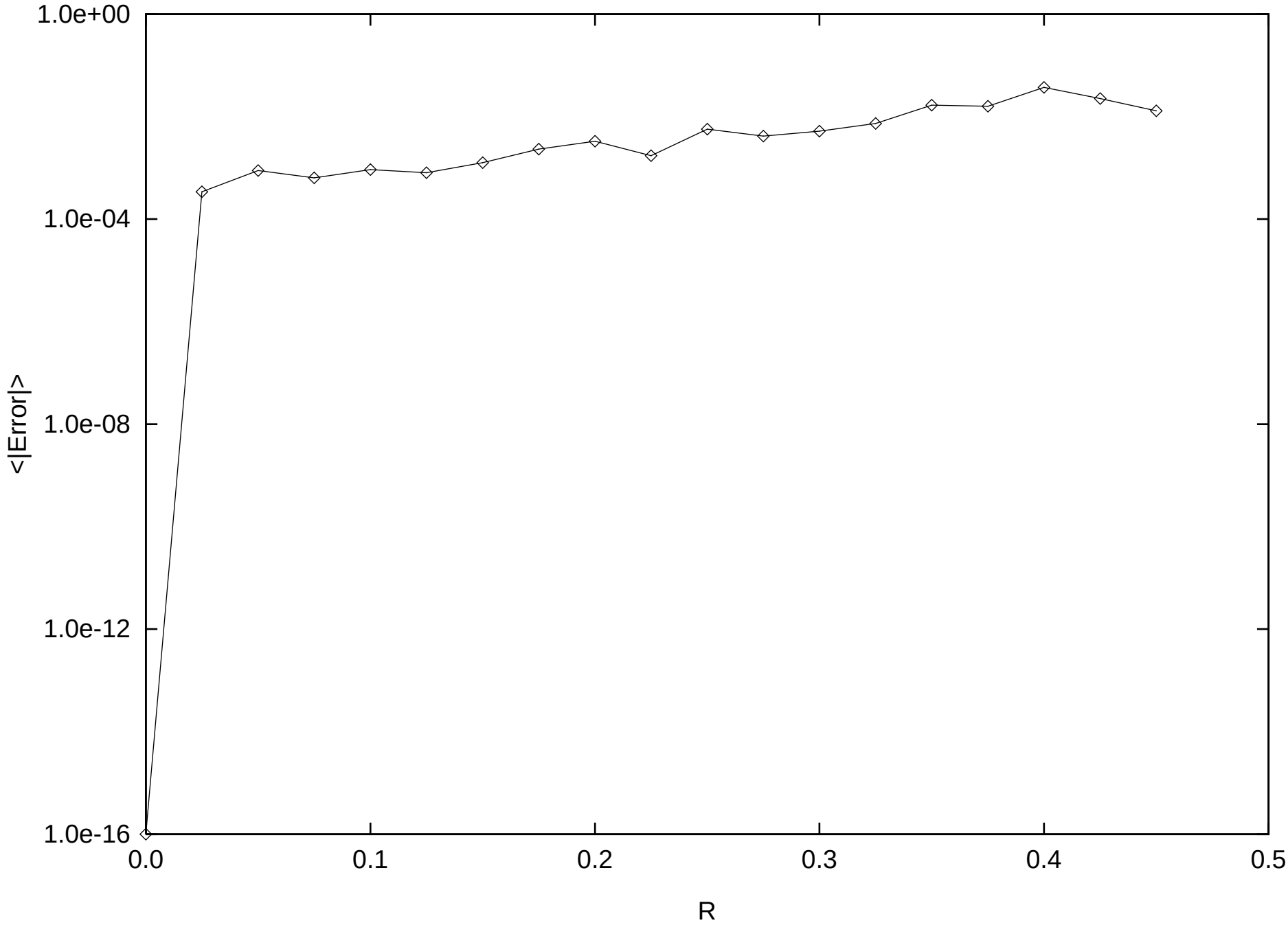
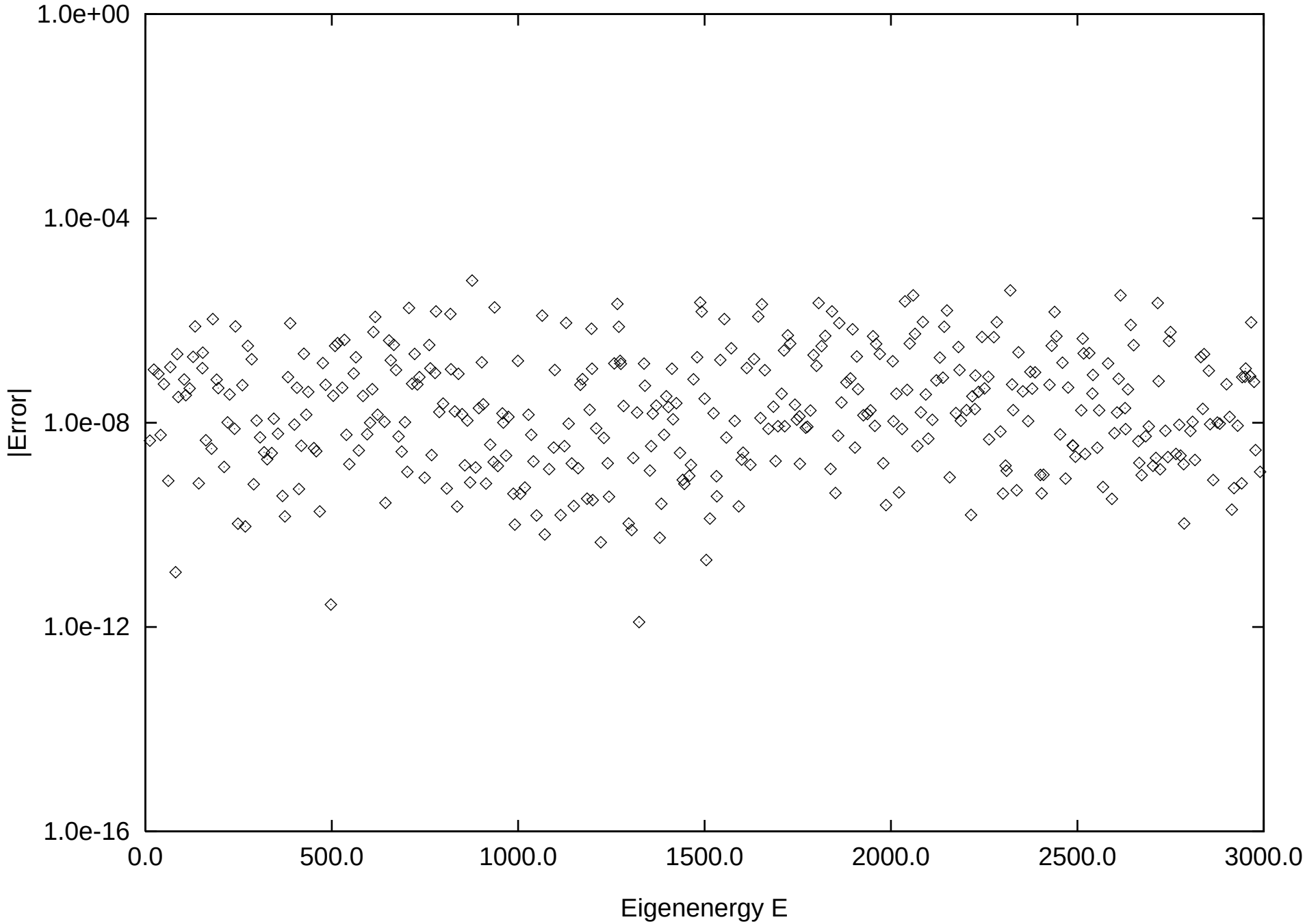


Figure 5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